

Spin glass behavior of the antiferromagnetic Heisenberg model on scale free network

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Abstract

Randomness and frustration are considered to be the key ingredients for the existence of spin glass (SG) phase. In a canonical system, these ingredients are realized by the random mixture of ferromagnetic (FM) and antiferromagnetic (AF) couplings. The study by Bartolozzi *et al.* [Phys. Rev. B **73**, 224419 (2006)] who observed the presence of SG phase on the AF Ising model on scale free network (SFN) is stimulating. It is a new type of SG system where randomness and frustration are not caused by the presence of FM and AF couplings. To further elaborate this type of system, here we study Heisenberg model on AF SFN and search for the SG phase. The canonical SG Heisenberg model is not observed in d -dimensional regular lattices for ($d \leq 3$). We can make an analogy for the connectivity density (m) of SFN with the dimensionality of the regular lattice. It should be plausible to find the critical value of m for the existence of SG behaviour, analogous to the lower critical dimension (d_l) for the canonical SG systems. Here we study system with $m = 2, 3, 4$ and 5. We used Replica Exchange algorithm of Monte Carlo Method and calculated the SG order parameter. We observed SG phase for each value of m and estimated its corresponding critical temperature.

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I. INTRODUCTION

Spin glass (SG) is one of the most complex systems in condensed matter physics and has been intensively studied in the last four decades[1–6]. It is a randomly frustrated magnetic system with frozen disordered spin orientation at low temperatures. This unusual configuration is regarded as a temporal ordered phase [7], different from the spatially ordered phase found in regular magnets. The complexity of the system is due to the presence of frustration and randomness, which are the key ingredients for the existence of SG phase. Frustration is a state where spins can not find fixed orientations to fully satisfy all the interactions with their neighboring spins. This can be caused either by the conflicting interaction between FM and AF couplings, or between among AF coupling due to the topological factors. Frustration alone can not lead a system to an SG phase, firmly exemplified by the fully frustrated AF planar spin systems which have spatially ordered phase at low temperatures[8, 9].

Most SGs studied are canonical system where both FM and AF couplings exist. The examples of these are Sherrington-Kirkpatrick model[2], Edward-Anderson model[3] and p-spin interaction model[4]. Bartolozzi *et al.* first reported SG behavior of the Ising model with AF interaction on scale free network (SFN)[10]. This is a new type of SG system without random distribution of FM and AF couplings. The nodes of the network do not have homogeneous number of links and frustration is fully due to the topological factor. The work has brought a new insight into the study of SGs, suggesting that the irregular connectivity can also be one of the ingredients of SGs, different from the previous notion insisting the presence of random mixture of FM and AF interactions.

An SFN consists of abundance of triangular units on which spins are frustrated if the couplings are AF. While the frustration is caused by the topological factor, the randomness is due to irregular connectivity. There are some vertices having very large number of connections, acting as the hubs as in the internet connection. In fact, the structure of the internet follows a scale free behavior. The AF Ising model on random networks without a scale free behavior was also reported to exhibit SG phase [11]. We believe that random connectivity can generally be an alternative for the usual randomness, together with frustration, as the ingredients of SGs.

Here we study the Heisenberg SG model on SFN. The prevalent controversy on existence of SG phase for the 3D canonical Heisenberg model [5] over the last three decades is one of the

main motivations. Most SGs studied, such as CuMn, AgMn or CdMnTe, are Heisenberg-like systems. Early numerical study by Coluzzi observed SG phase transition on 4D Heisenberg model. Kawamura and Nishikawa pointed out the absence of Heisenberg SG phase on D-dimensional space, for $D \leq 3$ [5]. These works suggested that the lower critical dimension d_l might be a fractional number, $3 < d_l < 4$.

For a regular lattice, spatial dimension is related to the coordination number, i.e., the number of neighbors of each spin. We can associate the coordination number with connectivity density m , which is the average number of links, of SFNs. Due to the presence of short-cut between spins, the notion of spatial dimension is not an appropriate term for SFNs. Nonetheless, an SFN can still be associated with a high dimensional regular lattice. Therefore, we assume that there may also be a critical value of m , analogous to d_l of regular lattice, for the random and SFNs. The paper is organized as follows: Section II describes the models and method. The results are discussed in Section III. Section IV is devoted for the summary and concluding remarks.

II. MODEL AND METHOD OF SIMULATION

The Heisenberg model on an SFN can be written with the following Hamiltonian,

$$H = -J \sum_{\langle ij \rangle} \vec{s}_i \cdot \vec{s}_j \quad (1)$$

where for an AF system, the coupling constant is set to be negative ($J < 0$); and \vec{s}_i are the Heisenberg spins residing on the nodes of the network. The summation is performed over all directly connected neighbors. In an SFN, the number of neighbors of each spin is not homogeneous. It is distinguished from a random network due to its scale free behavior, $P(k) = k^{-\gamma}$, where k is the number of links of each node and γ the decay exponent of its link distribution[12]. Networks with large γ have very famous nodes (or hubs), i.e., those having direct links to most other nodes. This type of network found many realizations in real world, from World Wide Webs, power grids, neural and cellular networks, till routers of the internet and citation network of scientists.

In addition, an SFN is also characterized by a clustering coefficient, C , defined as the average of local clustering, C_i ,

$$C_i = \frac{2y_i}{z_i(z_i - 1)} \quad (2)$$

where z_i is the total number of nodes linked to the i -th site and y_i is the total number of links connecting those nodes. Both C_i and C lie in the interval $[0,1]$. For a fully connected network, $C = C_i = 1$, all nodes connect to each other. The parameter C is related to the number or the density of triangles. Because spins on the vertices of triangular units are frustrated, C is also related to the frustration degree of the network. More comprehensive review on the ubiquitous of SFNs can be found for example in [13].

Thermal averages of the physical quantities of interest are calculated using the Replica Exchange algorithm of MC method[16]. This algorithm is implemented to overcome the slow dynamics due to the presence of local minima in the energy landscape of the system. Slow dynamics is a phenomenon commonly found in dealing with SGs, where a random walker can easily get trapped in one particular local minimum. It is an extended Metropolis algorithm where a system is duplicated into K replicas. All replicas are simulated in parallel and each is in equilibrium with a heat bath of an inverse temperature. Given K inverse temperatures, $\beta_1, \beta_2, \dots, \beta_K$, the probability distribution of finding the whole system in a state $\{X\} = \{X_1, X_2, \dots, X_K\}$ is given by,

$$P(\{X, \beta\}) = \prod_{m=1}^K \tilde{P}(X_m, \beta_m), \quad (3)$$

with

$$\tilde{P}(X_m, \beta_m) = Z(\beta_m)^{-1} \exp(-\beta_m H(X_m)), \quad (4)$$

and $Z(\beta_m)$ is the partition function of the m -th replica. We can define an exchange matrix between replicas as $W(X_m, \beta_m | X_n, \beta_n)$, which is the probability of switching configuration X_m at the temperature β_m with configuration X_n at β_n .

In order to keep the entire system at equilibrium, by using the detailed balance condition

$$\begin{aligned} & P(\dots, \{X_m, \beta_m\}, \dots, \{X_n, \beta_n\}, \dots) \cdot W(X_m, \beta_m | X_n, \beta_n) \\ &= P(\dots, \{X_n, \beta_n\}, \dots, \{X_m, \beta_m\}, \dots) \cdot W(X_n, \beta_n | X_m, \beta_m), \end{aligned} \quad (5)$$

along with Eq. (4), we have

$$\frac{W(X_m, \beta_m | X_n, \beta_n)}{W(X_n, \beta_n | X_m, \beta_m)} = \exp(-\Delta), \quad (6)$$

where $\Delta = (H(X_m) - H(X_n))(\beta_n - \beta_m)$. With the above constraint we can choose the

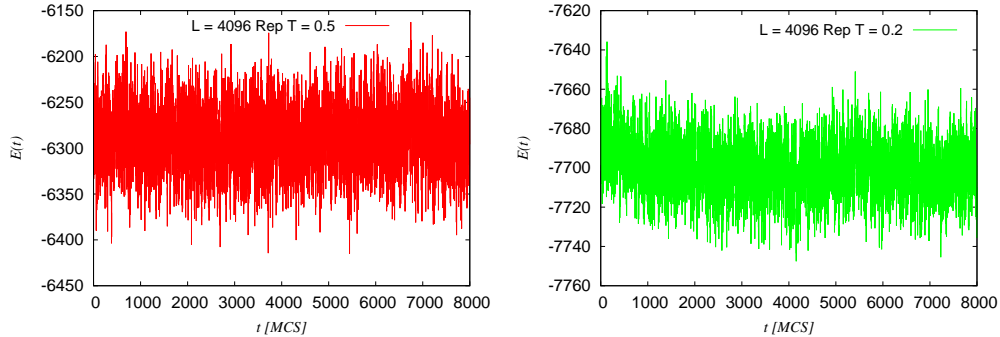


FIG. 1: Energy time series of system with $L = 4096$ and $m = 5$ at $T = 0.2$ and 0.5 .

matrix coefficients according to the standard Metropolis method, therefore

$$W(X_m, \beta_m | X_n, \beta_n) = \begin{cases} 1 & \text{if } \Delta \leq 0, \\ \exp(-\Delta) & \text{if Otherwise.} \end{cases} \quad (7)$$

As the acceptance ratio decays exponentially with $(\beta_n - \beta_m)$, the exchange is performed only to the replicas next to each other, i.e., $W(X_m, \beta_m | X_{m+1}, \beta_{m+1})$. The replica exchange method is extremely efficient for simulating systems such as SGs. This method has been widely implemented in many complex systems, including the AF-SFN Ising SG[10]. In the next section, we discuss the search for SG behaviour of Heisenberg antiferromagnetic system on SFN.

III. RESULTS AND DISCUSSION

A. Equilibrium Behavior

We have simulated AF Heisenberg model on SFN with various connectivity densities, $m = 2, 3, 4$ and 5 . For each density, we consider several system sizes, $L = 1024, 2048$, and 4096 , which are the number of spins. Since this is a random system, we took many realizations of the networks for each system size, then averaged the results over the number of realizations. Each realization corresponds to one particular connectivity distribution. We have to take reasonable number of realizations N_r for the better statistics of the results. Previous study on Ising system took $N_r = 1000$ realizations[10]. Here, due to the less fluctuation of the results from different realizations, we took moderate number of realizations, i.e., $N_r = 500$.

To check for the equilibrium behavior of the systems we evaluated the energy time series. In Monte Carlo (MC) simulation, time is assigned as a series of MC steps (MCSs). One MCS is defined as visiting each spin once, either randomly or consecutively, and performing a prescribed spin update, i.e., Metropolis update. We performed M MCSs for each temperature and took N samples out of M MCSs. The time series plot of energy for two different temperatures for system size $L = 4096$ is shown in Fig. 1. The phenomenon of slow dynamics at lower temperature ($T = 0.2$) is shown in Fig. 1 where the average value for the first half of the plot is larger than that of the rest half. To overcome this problem, the equilibration process was increased up to 8000 MCSs.

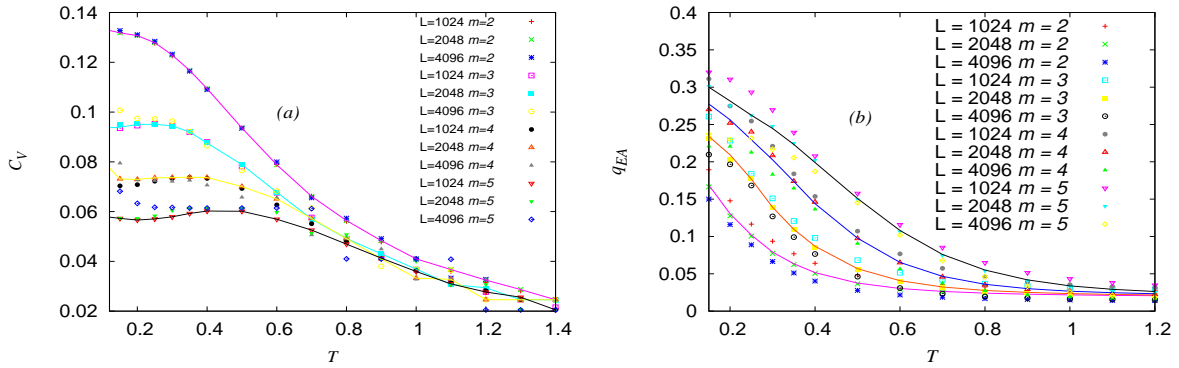


FIG. 2: Temperature dependence of (a) specific heat and (b) SG order parameter for different sizes with $m = 2, 3, 4$ and 5 . The solid lines are guides to the eye for the clarity of peaks.

We also calculated the specific heat which is defined as follows

$$C_v = \frac{N}{kT^2} (\langle E^2 \rangle - \langle E \rangle^2) \quad (8)$$

where L , k and $\langle E \rangle$ are respectively the number of nodes, Boltzmann constant and the ensemble average of energy. The temperature dependence of the specific heat for various system sizes is shown in Fig. 2(a), where the statistical errors are comparable to the size of the symbols. Although the specific heat plot exhibits no singularity, there is a maximum value at intermediate temperatures. As indicated, the peaks of the specific heat shift to higher temperatures as the increase in m . The presence of peak may signify the existence of phase transition. A clear sign of the SG phase can be observed from the plot of overlapping order parameter which will be presented in the next subsection.

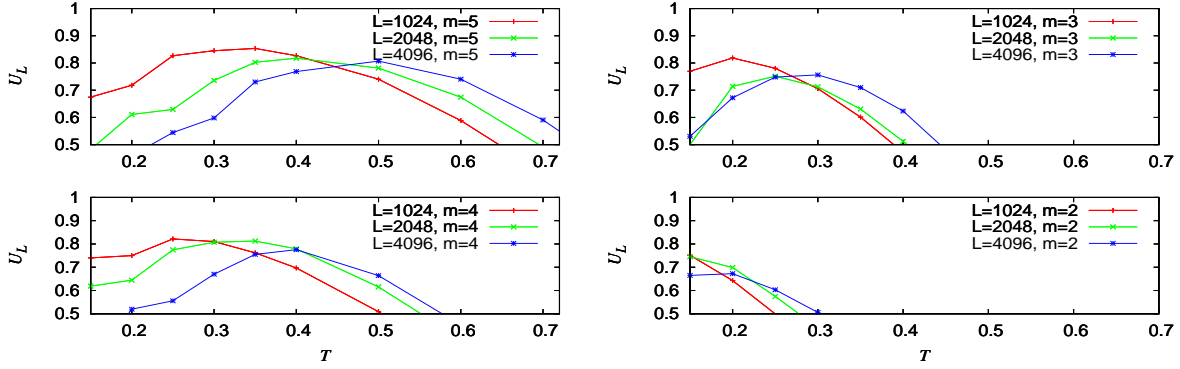


FIG. 3: Binder parameter of q_{EA} for various values of m . Solid lines are guide to the eyes.

B. Spin Glass Order Parameter

To search for the SG phase transition, we calculate SG order parameter defined as follows

$$q_{EA} = \left\langle \left| \sum_i \vec{s}_i^\alpha \otimes \vec{s}_i^\beta \right| \right\rangle_{av} \quad (9)$$

where \vec{s}_i is the spin on node i -th while α and β denote two sets of replicas. The origin of this quantity is from the scalar product of the vector spins. A scalar product of two vectors will be maximum (zero) if they are parallel (perpendicular). This idea is implemented to capture the frozeness of the spin configuration. If a system is frozen, the spin configurations of two replicas with the same inverse temperature from different sets will be more or less similar, regardless of globally rotational invariant. As explained in Sec. II, system is replicated into K replicas, each belongs to inverse temperature. For the sake of q_{EA} calculation, the whole replicas are duplicated, therefore we have two sets of replicas. Each set contains K replicas which are exchanged during the simulation. Only replicas from the same set were exchanged during the simulation.

The overlapping parameter will give finite value if system in SG phase. This applies for any SG model, including the Ising and the Heisenberg model. For Ising model, q_{EA} is simply the multiplication of the overlapped spins. In contrast for the Heisenberg model where spins are allowed to rotate in any direction, we take the tensor product instead of the scalar product, resulting q_{EA} with nine components. The plot of temperature dependence of q_{EA} for various different system sizes is shown in Fig. 2(b). As indicated, this parameter increases as temperature decreases, which is the evidence for the existence of SG phase at lower temperatures.

To clarify that this is a true SG phase, we calculate the cumulant ratio (Binder parameter) [18] of q_{EA} defined as follows

$$U_L = \frac{1}{2} \left[11 - \frac{9\langle q^4 \rangle}{\langle q^2 \rangle^2} \right] \quad (10)$$

The plot of U_L for different system sizes is shown in Fig. 3. It is clear that there is a single crossing point, emphasizing the existence of SG phase transition. However, due to the anomaly of the crossing pattern, which is different from the standard ones, such as in the previous study on Ising model[10], we did not perform scaling plot of U_L for the estimate of critical temperature and exponent. Instead, we roughly estimate the critical temperature for each connectivity density as listed in Table 1, where numbers in bracket are the uncertainty for the last digits. There is a systematic increase of critical temperature as the connectivity density increases. This is consistent with the Mean Field theory argument, where an ordered phase for a system with large connectivity tend to be more stable.

IV. SUMMARY AND CONCLUSION

In summary, we have studied AF Heisenberg model on scale free network, using Replica Exchange MC method. We simulated several different connectivity densities ($m = 2, 3, 4$ and 5) and calculated such physical quantities as ensemble average of energy, the specific heat, the overlapping parameter and its cumulant ratio (Binder parameter). A sign for finite SG phase transition was observed for all values of m . There is a systematic increase of T_c as m increases. This is related to the fact that systems with large connectivity tend to be more robust against thermal fluctuation. The existence of SG phase even in the system with $m = 2$ is generally in a good agreement with the case for canonical systems where Heisenberg SG phase was clearly observed in system with large dimension, e.g. the 4D system[14]. It is therefore interesting to search for the lower critical value of m by studying systems with fractional value of m . We will consider such system in our future study.

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TABLE I: The estimate of critical temperature T_c for each value of m .

Connectivity density (m)	T_c
5	0.44(3)
4	0.35(5)
3	0.24(6)
2	0.19(6)

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